



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2017 – 11:02 AM EDT

PDB ID : 5VEW
Title : Structure of the human GLP-1 receptor complex with PF-06372222
Authors : Song, G.; Yang, D.; Wang, Y.; Graaf, C.D.; Zhou, Q.; Jiang, S.; Liu, K.; Cai, X.; Dai, A.; Lin, G.; Liu, D.; Wu, F.; Wu, Y.; Zhao, S.; Ye, L.; Han, G.W.; Lau, J.; Wu, B.; Hanson, M.A.; Liu, Z.-J.; Wang, M.-W.; Stevens, R.C.
Deposited on : 2017-04-05
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

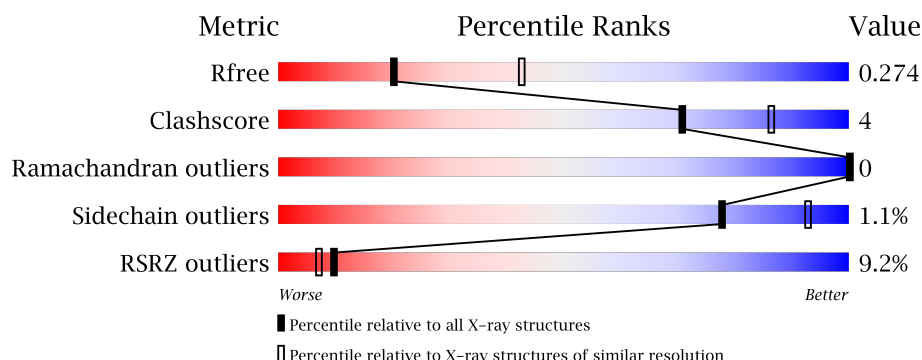
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	<div> <div>9%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	B	455	<div> <div>9%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLC	B	1203	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6849 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glucagon-like peptide 1 receptor,Endolysin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3302	2176	544	564	18			
1	B	424	Total	C	N	O	S	0	0	0
			3305	2176	548	563	18			

There are 48 discrepancies between the modelled and reference sequences:

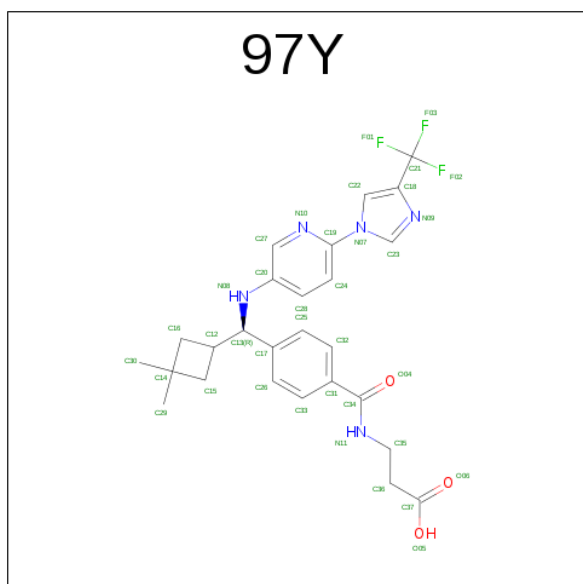
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	-	expression tag	UNP P43220
A	193	CYS	SER	ENGINEERED MUTATION	UNP P43220
A	196	PHE	ILE	ENGINEERED MUTATION	UNP P43220
A	212	GLY	TYR	linker	UNP P43220
A	?	-	THR	deletion	UNP P43220
A	?	-	ALA	deletion	UNP P43220
A	?	-	ALA	deletion	UNP P43220
A	?	-	GLN	deletion	UNP P43220
A	?	-	GLN	deletion	UNP P43220
A	?	-	HIS	deletion	UNP P43220
A	?	-	GLN	deletion	UNP P43220
A	214	GLY	TRP	linker	UNP P43220
A	225	ALA	SER	ENGINEERED MUTATION	UNP P43220
A	233	CSD	MET	ENGINEERED MUTATION	UNP P43220
A	1012	GLY	ARG	ENGINEERED MUTATION	UNP P00720
A	1054	THR	CYS	ENGINEERED MUTATION	UNP P00720
A	1097	ALA	CYS	ENGINEERED MUTATION	UNP P00720
A	1137	ARG	ILE	ENGINEERED MUTATION	UNP P00720
A	271	ALA	SER	ENGINEERED MUTATION	UNP P43220
A	317	CYS	ILE	ENGINEERED MUTATION	UNP P43220
A	318	ILE	GLY	ENGINEERED MUTATION	UNP P43220
A	346	ALA	LYS	ENGINEERED MUTATION	UNP P43220
A	347	PHE	CYS	ENGINEERED MUTATION	UNP P43220
A	361	CYS	GLY	ENGINEERED MUTATION	UNP P43220
B	127	SER	-	expression tag	UNP P43220

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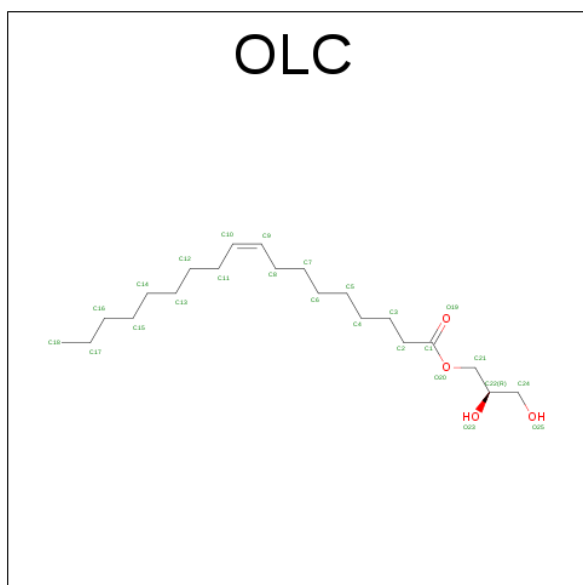
Chain	Residue	Modelled	Actual	Comment	Reference
B	193	CYS	SER	ENGINEERED MUTATION	UNP P43220
B	196	PHE	ILE	ENGINEERED MUTATION	UNP P43220
B	212	GLY	TYR	linker	UNP P43220
B	?	-	THR	deletion	UNP P43220
B	?	-	ALA	deletion	UNP P43220
B	?	-	ALA	deletion	UNP P43220
B	?	-	GLN	deletion	UNP P43220
B	?	-	GLN	deletion	UNP P43220
B	?	-	HIS	deletion	UNP P43220
B	?	-	GLN	deletion	UNP P43220
B	214	GLY	TRP	linker	UNP P43220
B	225	ALA	SER	ENGINEERED MUTATION	UNP P43220
B	233	CSD	MET	ENGINEERED MUTATION	UNP P43220
B	1012	GLY	ARG	ENGINEERED MUTATION	UNP P00720
B	1054	THR	CYS	ENGINEERED MUTATION	UNP P00720
B	1097	ALA	CYS	ENGINEERED MUTATION	UNP P00720
B	1137	ARG	ILE	ENGINEERED MUTATION	UNP P00720
B	271	ALA	SER	ENGINEERED MUTATION	UNP P43220
B	317	CYS	ILE	ENGINEERED MUTATION	UNP P43220
B	318	ILE	GLY	ENGINEERED MUTATION	UNP P43220
B	346	ALA	LYS	ENGINEERED MUTATION	UNP P43220
B	347	PHE	CYS	ENGINEERED MUTATION	UNP P43220
B	361	CYS	GLY	ENGINEERED MUTATION	UNP P43220

- Molecule 2 is N-{4-[(R)-(3,3-dimethylcyclobutyl)({6-[4-(trifluoromethyl)-1H-imidazol-1-yl]pyridin-3-yl}amino)methyl]benzene-1-carbonyl}-beta-alanine (three-letter code: 97Y) (formula: C₂₆H₂₈F₃N₅O₃).



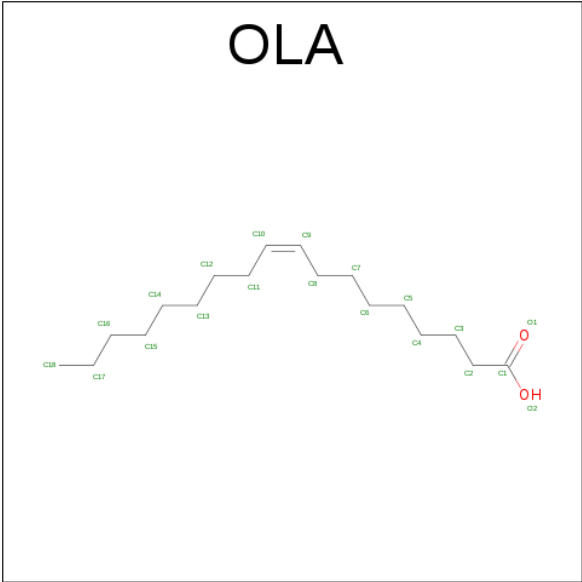
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			37	26	3	5	3		
2	B	1	Total	C	F	N	O	0	0
			37	26	3	5	3		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			19	15	4		
3	B	1	Total	C	O	0	0
			25	21	4		
3	B	1	Total	C	O	0	0
			19	15	4		
3	B	1	Total	C	O	0	0
			15	11	4		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		

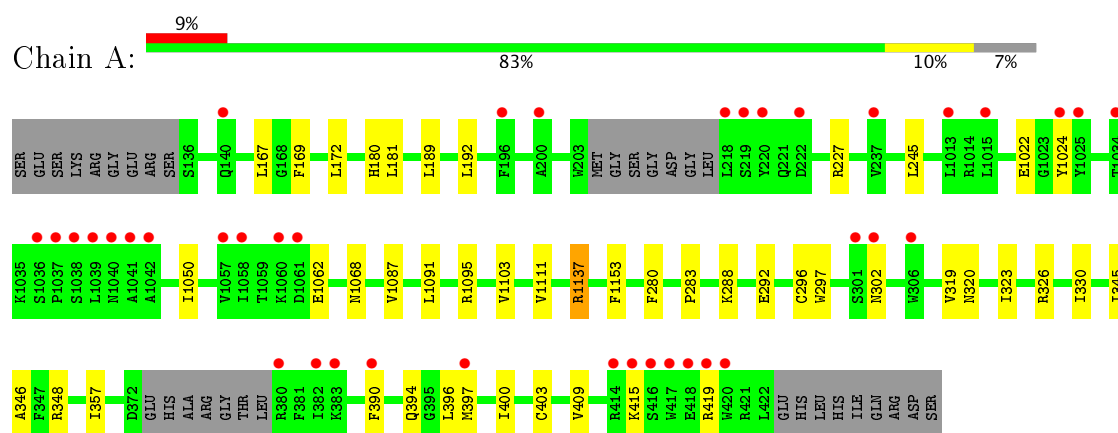
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	7	Total	O	0	0
			7	7		

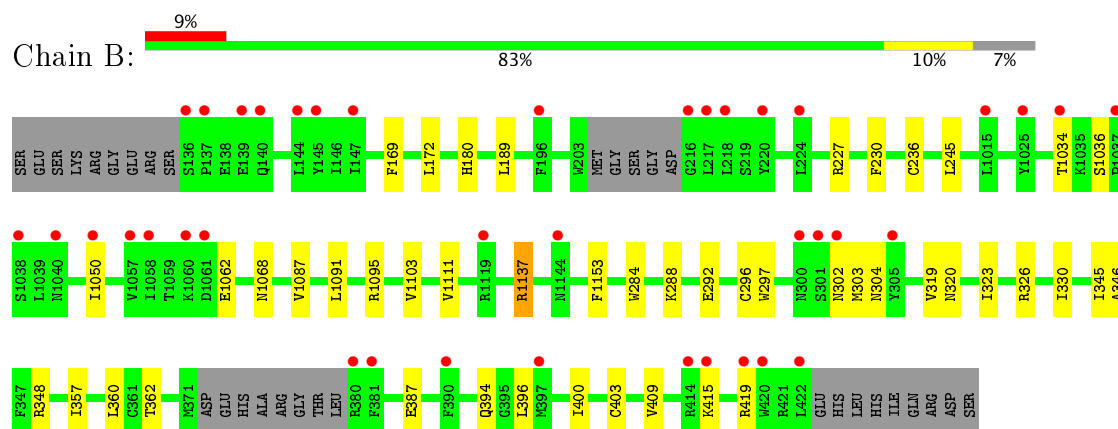
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glucagon-like peptide 1 receptor,Endolysin chimera



- Molecule 1: Glucagon-like peptide 1 receptor,Endolysin chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.77Å 66.43Å 83.44Å 90.54° 90.18° 107.73°	Depositor
Resolution (Å)	30.00 – 2.70 29.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-2.70) 94.8 (29.73-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.68Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.228 , 0.246 0.259 , 0.274	Depositor DCC
R_{free} test set	1742 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6849	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, OLC, 97Y, OLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3371	0.55	0/4590
1	B	0.51	0/3374	0.57	0/4593
All	All	0.51	0/6745	0.56	0/9183

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3302	0	3250	27	0
1	B	3305	0	3251	29	0
2	A	37	0	0	1	0
2	B	37	0	0	1	0
3	A	44	0	65	1	0
3	B	84	0	124	2	0
4	A	20	0	33	1	0
5	A	13	0	0	0	0
5	B	7	0	0	0	0
All	All	6849	0	6723	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 4.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:MET:HG2	1:B:304:ASN:H	1.45	0.79
1:A:1050:ILE:HD11	1:A:1062:GLU:HB3	1.73	0.69
1:B:1050:ILE:HD11	1:B:1062:GLU:HB3	1.74	0.69
1:B:387:GLU:HG3	3:B:1203:OLC:H17A	1.79	0.64
1:B:360:LEU:HG	1:B:394:GLN:HE21	1.67	0.60
1:B:288:LYS:HE3	1:B:297:TRP:HB3	1.83	0.59
1:A:403:CYS:O	1:A:409:VAL:HG21	2.06	0.55
1:A:390:PHE:O	1:A:394:GLN:HG3	2.06	0.54
1:B:403:CYS:O	1:B:409:VAL:HG21	2.08	0.54
1:A:292:GLU:OE2	1:A:302:ASN:HB3	2.09	0.52
1:B:227:ARG:HG2	1:B:296:CYS:HA	1.92	0.52
1:B:415:LYS:O	1:B:419:ARG:HG2	2.11	0.51
1:A:415:LYS:O	1:A:419:ARG:HG2	2.11	0.50
1:A:1095:ARG:HG2	1:A:1153:PHE:HA	1.94	0.50
1:B:1095:ARG:HG2	1:B:1153:PHE:HA	1.94	0.50
1:A:396:LEU:O	1:A:400:ILE:HG12	2.12	0.49
1:B:1034:THR:HG22	1:B:1036:SER:H	1.77	0.49
1:B:292:GLU:OE2	1:B:302:ASN:HB3	2.13	0.48
1:A:167:LEU:HD22	4:A:1204:OLA:H42	1.96	0.47
1:B:396:LEU:O	1:B:400:ILE:HG12	2.14	0.47
1:A:288:LYS:CE	1:A:297:TRP:HB3	2.44	0.47
1:B:1095:ARG:HD3	1:B:1153:PHE:O	2.16	0.46
1:A:1095:ARG:HD3	1:A:1153:PHE:O	2.16	0.46
1:B:362:THR:CG2	3:B:1203:OLC:H12	2.45	0.46
1:A:348:ARG:HB3	2:A:1201:97Y:C36	2.45	0.46
1:B:348:ARG:HB3	2:B:1202:97Y:C36	2.46	0.46
1:A:181:LEU:HB3	3:A:1202:OLC:H4	1.98	0.46
1:B:1103:VAL:HG22	1:B:1111:VAL:HG21	1.98	0.46
1:A:1103:VAL:HG22	1:A:1111:VAL:HG21	1.99	0.45
1:A:227:ARG:HG2	1:A:296:CYS:HA	1.99	0.44
1:B:288:LYS:O	1:B:297:TRP:CE2	2.71	0.44
1:A:326:ARG:O	1:A:330:ILE:HG12	2.18	0.43
1:A:169:PHE:HB2	1:A:172:LEU:HD12	2.01	0.42
1:A:280:PHE:C	1:A:283:PRO:HD2	2.40	0.42
1:B:326:ARG:O	1:B:330:ILE:HG12	2.19	0.42
1:A:345:ILE:HG13	1:A:346:ALA:N	2.35	0.42
1:B:288:LYS:HD2	1:B:292:GLU:HB2	2.01	0.42
1:A:288:LYS:HE3	1:A:297:TRP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ARG:HB3	1:B:297:TRP:CZ2	2.55	0.42
1:B:169:PHE:HB2	1:B:172:LEU:HD12	2.02	0.42
1:B:1087:VAL:O	1:B:1091:LEU:HG	2.20	0.41
1:A:1087:VAL:O	1:A:1091:LEU:HG	2.20	0.41
1:A:1137:ARG:H	1:A:1137:ARG:HD3	1.84	0.41
1:A:245:LEU:HD13	1:A:319:VAL:HG23	2.02	0.41
1:B:345:ILE:HG13	1:B:346:ALA:N	2.36	0.41
1:A:320:ASN:HB3	1:A:357:ILE:HG23	2.02	0.41
1:A:319:VAL:O	1:A:323:ILE:HG12	2.21	0.41
1:B:245:LEU:HD13	1:B:319:VAL:HG23	2.03	0.41
1:B:189:LEU:HB3	1:B:236:CYS:SG	2.60	0.41
1:A:288:LYS:HE2	1:A:297:TRP:HB3	2.03	0.41
1:B:319:VAL:O	1:B:323:ILE:HG12	2.21	0.41
1:B:1137:ARG:H	1:B:1137:ARG:HD3	1.85	0.41
1:B:230:PHE:CE2	1:B:284:TRP:HH2	2.39	0.41
1:A:189:LEU:HA	1:A:192:LEU:HD12	2.02	0.40
1:B:320:ASN:HB3	1:B:357:ILE:HG23	2.03	0.40
1:A:1022:GLU:HB2	1:A:1024:TYR:HD1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	416/455 (91%)	392 (94%)	24 (6%)	0	100	100
1	B	417/455 (92%)	391 (94%)	26 (6%)	0	100	100
All	All	833/910 (92%)	783 (94%)	50 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/394 (84%)	326 (99%)	4 (1%)	75	92
1	B	329/394 (84%)	326 (99%)	3 (1%)	82	94
All	All	659/788 (84%)	652 (99%)	7 (1%)	78	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	HIS
1	A	1068	ASN
1	A	1137	ARG
1	A	397	MET
1	B	180	HIS
1	B	1068	ASN
1	B	1137	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	1068	ASN
1	B	240	ASN
1	B	1068	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CSD	A	233	1	4,7,8	1.29	1 (25%)	2,8,10	3.21	1 (50%)
1	CSD	B	233	1	4,7,8	1.42	1 (25%)	2,8,10	3.00	2 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	233	1	-	0/2/6/8	0/0/0/0
1	CSD	B	233	1	-	1/2/6/8	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	CSD	CA-C	2.23	1.53	1.50
1	B	233	CSD	CA-C	2.51	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	CSD	O-C-CA	-2.00	119.48	125.02
1	B	233	CSD	OD1-SG-CB	3.74	112.61	105.61
1	A	233	CSD	OD1-SG-CB	4.10	113.29	105.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	233	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	97Y	A	1201	-	35,40,40	2.17	10 (28%)	47,59,59	1.81	9 (19%)
3	OLC	A	1202	-	24,24,24	1.01	1 (4%)	25,25,25	1.00	2 (8%)
3	OLC	A	1203	-	18,18,24	1.14	1 (5%)	19,19,25	0.98	1 (5%)
4	OLA	A	1204	-	16,19,19	0.24	0	15,19,19	0.58	0
3	OLC	B	1201	-	24,24,24	0.98	1 (4%)	25,25,25	0.95	2 (8%)
2	97Y	B	1202	-	35,40,40	2.18	10 (28%)	47,59,59	1.82	9 (19%)
3	OLC	B	1203	-	24,24,24	0.99	1 (4%)	25,25,25	0.87	1 (4%)
3	OLC	B	1204	-	18,18,24	1.09	1 (5%)	19,19,25	0.90	1 (5%)
3	OLC	B	1205	-	14,14,24	1.26	1 (7%)	15,15,25	1.20	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	97Y	A	1201	-	-	0/26/42/42	0/4/4/4
3	OLC	A	1202	-	-	0/24/24/24	0/0/0/0
3	OLC	A	1203	-	-	0/18/18/24	0/0/0/0
4	OLA	A	1204	-	-	0/15/17/17	0/0/0/0
3	OLC	B	1201	-	-	0/24/24/24	0/0/0/0
2	97Y	B	1202	-	-	0/26/42/42	0/4/4/4
3	OLC	B	1203	-	-	0/24/24/24	0/0/0/0
3	OLC	B	1204	-	-	0/18/18/24	0/0/0/0
3	OLC	B	1205	-	-	0/14/14/24	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	97Y	C22-N07	-5.93	1.32	1.39
2	B	1202	97Y	C22-N07	-5.82	1.32	1.39
2	A	1201	97Y	C15-C12	-3.48	1.50	1.55
2	B	1202	97Y	C15-C12	-3.47	1.51	1.55
2	B	1202	97Y	C12-C13	-3.04	1.48	1.53
2	A	1201	97Y	C12-C13	-3.04	1.48	1.53
2	A	1201	97Y	C16-C14	-2.94	1.51	1.55
2	B	1202	97Y	C16-C12	-2.87	1.51	1.55
2	A	1201	97Y	C16-C12	-2.84	1.51	1.55
2	B	1202	97Y	C16-C14	-2.83	1.51	1.55
2	B	1202	97Y	C15-C14	-2.37	1.51	1.55
2	A	1201	97Y	C15-C14	-2.28	1.52	1.55
2	B	1202	97Y	C19-N07	2.62	1.46	1.43
2	A	1201	97Y	C19-N07	2.73	1.46	1.43
2	A	1201	97Y	C17-C13	2.90	1.55	1.51
2	B	1202	97Y	C17-C13	3.00	1.55	1.51
2	B	1202	97Y	C20-N08	3.52	1.46	1.39
2	A	1201	97Y	C20-N08	3.56	1.46	1.39
3	B	1204	OLC	O20-C1	4.29	1.46	1.33
3	B	1201	OLC	O20-C1	4.45	1.46	1.33
3	B	1205	OLC	O20-C1	4.48	1.46	1.33
3	B	1203	OLC	O20-C1	4.55	1.46	1.33
3	A	1203	OLC	O20-C1	4.57	1.46	1.33
3	A	1202	OLC	O20-C1	4.59	1.46	1.33
2	A	1201	97Y	C34-N11	5.58	1.46	1.33
2	B	1202	97Y	C34-N11	5.72	1.46	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	97Y	C17-C13-C12	-5.33	107.26	112.18
2	A	1201	97Y	C17-C13-C12	-5.29	107.30	112.18
2	A	1201	97Y	C24-C19-N10	-4.61	119.53	125.48
2	B	1202	97Y	C24-C19-N10	-4.48	119.70	125.48
2	B	1202	97Y	C20-C27-N10	-2.85	121.65	124.25
2	A	1201	97Y	C24-C28-C20	-2.60	117.25	120.30
2	A	1201	97Y	C20-C27-N10	-2.59	121.89	124.25
2	B	1202	97Y	C24-C28-C20	-2.46	117.41	120.30
2	B	1202	97Y	F02-C21-C18	-2.41	108.39	112.46
3	B	1205	OLC	O20-C1-O19	-2.30	117.84	123.55
3	B	1201	OLC	O20-C1-O19	-2.28	117.89	123.55
3	A	1202	OLC	O20-C1-O19	-2.26	117.95	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	97Y	F03-C21-C18	-2.12	108.88	112.46
2	A	1201	97Y	F03-C21-C18	-2.11	108.89	112.46
2	A	1201	97Y	F02-C21-C18	-2.06	108.98	112.46
2	A	1201	97Y	C27-N10-C19	2.20	121.42	117.37
2	B	1202	97Y	C27-N10-C19	2.30	121.61	117.37
3	B	1204	OLC	O20-C1-C2	2.62	119.52	111.90
3	B	1203	OLC	O20-C1-C2	2.78	120.00	111.90
2	B	1202	97Y	C28-C24-C19	2.93	120.58	116.66
3	A	1203	OLC	O20-C1-C2	2.93	120.43	111.90
3	B	1201	OLC	O20-C1-C2	3.03	120.71	111.90
3	B	1205	OLC	O20-C1-C2	3.11	120.95	111.90
3	A	1202	OLC	O20-C1-C2	3.17	121.13	111.90
2	A	1201	97Y	C28-C24-C19	3.20	120.94	116.66
2	A	1201	97Y	C21-C18-N09	6.12	126.96	119.76
2	B	1202	97Y	C21-C18-N09	6.21	127.07	119.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	97Y	1	0
3	A	1202	OLC	1	0
4	A	1204	OLA	1	0
2	B	1202	97Y	1	0
3	B	1203	OLC	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/455 (92%)	0.54	39 (9%) 10 7	63, 99, 159, 185	0
1	B	423/455 (92%)	0.51	39 (9%) 10 7	63, 96, 158, 185	0
All	All	845/910 (92%)	0.52	78 (9%) 10 7	63, 97, 159, 185	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1037	PRO	12.6
1	A	218	LEU	8.6
1	A	302	ASN	7.9
1	A	1037	PRO	6.3
1	A	1040	ASN	6.0
1	B	422	LEU	5.9
1	B	216	GLY	5.9
1	B	1038	SER	5.8
1	B	302	ASN	5.6
1	B	217	LEU	5.3
1	A	1038	SER	4.5
1	B	1040	ASN	4.4
1	A	419	ARG	4.4
1	A	418	GLU	4.3
1	B	414	ARG	3.8
1	B	140	GLN	3.7
1	A	301	SER	3.6
1	A	416	SER	3.6
1	B	380	ARG	3.4
1	A	219	SER	3.4
1	A	1057	VAL	3.4
1	A	220	TYR	3.4
1	A	1025	TYR	3.3
1	B	305	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1061	ASP	3.3
1	B	144	LEU	3.3
1	B	196	PHE	3.2
1	A	397	MET	3.2
1	B	419	ARG	3.1
1	B	1057	VAL	3.0
1	A	1024	TYR	2.9
1	B	1025	TYR	2.9
1	A	306	TRP	2.9
1	A	414	ARG	2.8
1	A	1015	LEU	2.8
1	A	382	ILE	2.8
1	A	390	PHE	2.7
1	A	417	TRP	2.7
1	A	415	LYS	2.7
1	A	1034	THR	2.7
1	B	397	MET	2.7
1	B	1061	ASP	2.7
1	B	147	ILE	2.6
1	B	224	LEU	2.5
1	B	415	LYS	2.5
1	A	1041	ALA	2.5
1	A	1060	LYS	2.4
1	A	1039	LEU	2.4
1	B	139	GLU	2.4
1	B	381	PHE	2.3
1	B	137	PRO	2.3
1	A	420	TRP	2.3
1	B	145	TYR	2.3
1	B	1015	LEU	2.3
1	A	140	GLN	2.3
1	A	380	ARG	2.3
1	A	1058	ILE	2.3
1	B	301	SER	2.3
1	B	1058	ILE	2.3
1	B	1119	ARG	2.2
1	B	1050	ILE	2.2
1	A	1013	LEU	2.2
1	B	300	ASN	2.2
1	B	420	TRP	2.2
1	A	237	VAL	2.2
1	A	200	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	136	SER	2.1
1	A	196	PHE	2.1
1	B	1060	LYS	2.1
1	B	218	LEU	2.1
1	A	383	LYS	2.1
1	A	222	ASP	2.1
1	B	390	PHE	2.1
1	B	1034	THR	2.1
1	A	1036	SER	2.0
1	A	1042	ALA	2.0
1	B	220	TYR	2.0
1	B	1144	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	A	233	8/9	0.87	0.26	-	93,95,101,101	0
1	CSD	B	233	8/9	0.84	0.23	-	86,91,97,97	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	OLC	B	1203	25/25	0.65	0.31	2.74	95,99,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	OLC	B	1201	25/25	0.75	0.29	1.79	104,110,113,114	0
3	OLC	A	1202	25/25	0.81	0.23	1.15	109,112,115,116	0
3	OLC	B	1205	15/25	0.65	0.20	0.99	137,141,143,143	0
2	97Y	B	1202	37/37	0.96	0.19	0.07	74,89,105,106	0
3	OLC	B	1204	19/25	0.83	0.18	0.07	114,115,118,120	0
2	97Y	A	1201	37/37	0.95	0.18	-0.20	83,95,108,109	0
3	OLC	A	1203	19/25	0.75	0.16	-0.83	142,145,152,153	0
4	OLA	A	1204	20/20	0.69	0.37	-	131,135,140,141	0

6.5 Other polymers

There are no such residues in this entry.